



**Jeffrey P. Greeley**  
*Assistant Scientist*

Theme: Theory and Modeling  
Phone: (630) 252-4711  
Fax: (630) 252-4646  
Email: [jgreeley@anl.gov](mailto:jgreeley@anl.gov)

Argonne National Laboratory  
Center for Nanoscale Materials  
9700 S. Cass Ave.  
Argonne, IL 60439

**Research summary:**

Our current research focuses on the use of Density Functional Theory techniques to understand the kinetics and thermodynamics of chemical reactions on nanostructured metal and oxide surfaces. We aim to develop models of reactions relevant to heterogeneous catalysis and to electrocatalysis; in tandem, we will develop computational screening techniques that will permit the efficient design of new catalytic materials from first principles. Selected reactions of interest include the CO electrooxidation reaction, the selective, oxidative dehydrogenation of propane to propene, and the electrooxidation of small organic molecules; these reactions play an important role in the operation of fuel cells and in the production of useful chemical compounds from raw hydrocarbon feedstocks. A related interest is the development of new, first principles-based techniques to model the dissolution and corrosion of metallic surfaces; this research is related to the development both of catalysts that are stable in electrochemical environments and of corrosion-resistant surfaces.

**Selected recent publications:**

1. "Trends in Particle Size Effects for the Oxygen Reduction Reaction." J. Greeley, J. Rossmeisl, A. Hellman, J. K. Nørskov, *submitted*.
2. "Scaling Properties of Adsorption Energies for Molecules on Transition Metal Surfaces", F. Abild-Pedersen, J. Greeley, F. Studt, J. Rossmeisl, T. R. Munter, P.G. Moses, T. Bligaard, and J. K. Nørskov, *Physical Review Letters*, *accepted*.
3. "Electrochemical Dissolution of Surface Alloys in Acids: Thermodynamic Trends for First-Principles Calculations." J. Greeley and J. K. Nørskov, *Electrochimica Acta*, **52** (2007) 5829.
4. "Computational High-Throughput Screening of Electrocatalytic Materials for Hydrogen Evolution." J. Greeley, T. Jaramillo, J. Bonde, I. Chorkendorff, and J. Nørskov, *Nature Materials*, **5**, 909 (2006).
5. "Changing the Activity of Electrocatalysts for Oxygen Reduction by Tuning the Surface Electronic Structure." V. Stamenkovic, B. S. Moon, K. J. J. Mayrhofer, P. N. Ross, N. M. Markovic, J. Rossmeisl, J. Greeley, and J. K. Nørskov, *Angewandte Chemie International Edition (cover page)*, **45**, 2897 (2006).